

Self-organization of irregular NEM vibrations in multi-mode shuttle structures

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We investigate theoretically multi-mode electromechanical “shuttle” instabilities in DC voltage-biased nanoelectromechanical single-electron tunneling (NEM-SET) devices. We show that initially irregular (quasi-periodic) oscillations, that occur as a result of the simultaneous self-excitation of several mechanical modes with incommensurable frequencies, self-organize into periodic oscillations with a frequency corresponding to the eigenfrequency of one of the unstable modes. This effect demonstrates that a local probe can selectively excite global vibrations of extended objects.

PACS numbers: 85.35.Kt, 85.85.+j

In a nanoelectromechanical single-electron tunneling (NEM-SET) device mechanical vibrations and single-electron tunneling events are coupled on the nanometer length scale. Ten years ago Gorelik *et al.* [1] suggested that such a coupling of mechanical and electrical degrees of freedom could lead to a “shuttle instability” and to a novel shuttle mechanism for charge transport through a DC voltage-biased NEM-SET. The theory [1] was developed for a rigid nanometer-size metal cluster suspended by elastic links between a source and a drain electrode so that only one mechanical degree of freedom was involved. Internal cluster vibrations were assumed to have much higher frequencies than the relatively low-frequency center-of-mass vibration and were therefore ignored. In the proposed shuttle regime charge transport between source and drain is mechanically assisted by pronounced center-of-mass vibrations of the cluster (for reviews see [2, 3]).

In this Letter — motivated by the recent experimental discovery of the shuttle instability predicted in Ref. [1] and of the related self excitation of radio-frequency mechanical vibrations of gold-capped silicon nano-pillars [4] — we generalize the theory of the shuttle phenomenon to include extended structures with (many) internal mechanical degrees of freedom. Our objective is to stimulate further experimental work on NEM-SET systems involving, *e.g.*, suspended carbon nanotubes and other extended molecules. In many such systems internal mechanical degrees of freedom cannot be ignored and therefore a theory of shuttling in the multi-mode regime needs to be developed. This will be done in what follows.

Our main result is that when self excitation involves more than one mode, strong mode-mode interactions caused by the non-linear coupling of the mechanical vibrations to the electronic subsystem results in self-organization of the vibrations. This implies that initially quasi-periodic vibrations are transformed into pronounced periodic vibrations as the shuttle instability develops towards a steady state. The frequency of the steady-state vibrations depends crucially on initial conditions and corresponds to the eigenfrequency of one of

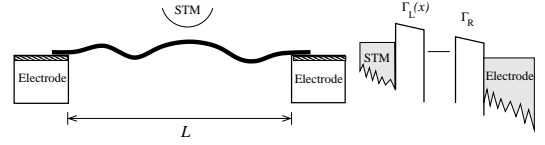


Figure 1: Sketch of the model system considered. The electron tunneling rate $\Gamma_L(x)$ between the STM-tip and the center of a suspended carbon nanotube depends on the tube position, while the tunneling rate Γ_R between tube and electrodes is constant. Tunneling may lead to self-excitation of multiple nanotube bending modes, which self-organize into periodic, single-mode oscillations (the vibration amplitude shown is exaggerated).

the unstable modes.

We will consider the particular realization of a multi-mode shuttle structure sketched in Fig. 1. The sketch shows a NEM-SET device based on a carbon nanotube (CNT) suspended over a trench so that a segment of the tube is free to move in response to external forces. Charge is injected into the suspended nanotube through the tip of a scanning tunneling microscope (STM) positioned above the center of the tube [5] as in the experiment of LeRoy *et al.* [6]. For this very system a current driven nanoelectromechanical instability has been predicted and theoretically shown to result in the onset of pronounced CNT bending mode vibrations involving one or more modes [7, 8]. Below we will consider the detailed development of the predicted instability when several bending modes are unstable in order to find the resulting steady state. While a nanoelectromechanical instability involving these modes has not yet been observed experimentally, bending mode vibrations of suspended CNTs have been detected in devices of the type studied here [9, 10]. We note in passing that the electromechanical coupling to other types of CNT vibration modes have also been studied [6, 11, 12, 13, 14].

We use continuum elasticity theory to describe the nanotube mechanics [15, 16]. The set of normal modes for the bending mode vibrations is characterized by the fre-

quencies $\omega_n = \frac{c_n}{L^2} \sqrt{\frac{EI_z}{\rho S}}$, where E is Young's modulus of the CNT, I_z is the area moment of inertia of the cross section, ρ is the mass density, S is the cross section area and the coefficients $c_n = 22.4, 61.7, 120.9, 199.9, 298.6, \dots$ are obtained by solving the equation $\cos \sqrt{c_n} \cosh \sqrt{c_n} = 1$ [17]. The displacement $x(t)$ of the center of the CNT (see Fig. 1) can be expressed as a sum of normal-mode amplitudes $x_n(t)$, where only modes with $n = 1, 3, 5, \dots$ contribute due to symmetry. Other modes are inert and can be neglected. Each normal mode coordinate x_n obeys Newton's equation in the form

$$\ddot{x}_n + \gamma \dot{x}_n + \omega_n^2 x_n = q\mathcal{E}/M, \quad (1)$$

where the force term depends on the average net charge q on the CNT and the effective electric field \mathcal{E} that acts on the tube as a result of the applied bias voltage [7]. The damping coefficient γ in Eq. (1) is a constant in our model and therefore affects all modes in the same way. It is related to the quality factor of the vibration modes through the relation $Q_n = \omega_n/\gamma$. Experimentally Q factors of order 1000 have been reported for nanoscale CNT based resonators in vacuum, [18], while Q factors as high as $10^4 - 10^5$ have been found for somewhat larger Si [19] and SiC resonators [20].

An important parameter for the system under consideration is the ratio ω/Γ between the typical CNT vibration frequency ω and the characteristic rate of electron tunneling Γ . Having in mind that the mechanical vibration frequency is extremely low on an electronic scale ($\omega \sim 10^8 - 10^9 \text{ s}^{-1}$ for $L \simeq 1 \mu\text{m}$) we consider here the case $\omega \ll \Gamma$. In addition we focus on the single-electron shuttling regime, where only one electron can be accumulated on the CNT due to Coulomb blockade of tunneling. Introducing the probability p to find an extra electron on the nanotube the average excess charge is $q = ep$ while the kinetic equation for the time evolution of the probability p can be written as

$$\dot{p} = -\Gamma(x)p + \Gamma_L(x). \quad (2)$$

Here $\Gamma(x) = \Gamma_L(x) + \Gamma_R$ with $x = \sum_n x_n$ while $\Gamma_L(x) = \Gamma_0 \exp(-x/\lambda)$ is the rate of electron tunneling across the STM-CNT junction, so that the typical rate of electron tunneling is $\Gamma \equiv \Gamma_0 + \Gamma_R$. The characteristic length λ is known as the tunneling length.

Equations (1) and (2) describe the coupled nanoelectromechanical dynamics of the CNT-based NEM-SET device. In order to stay in the single-electron shuttling regime one has to apply a small enough bias voltage: 0.1 V is a typical value for a CNT of length $L \simeq 1 \mu\text{m}$. Therefore, it is reasonable to consider the limit of weak nanoelectromechanical coupling where the tunneling rates are only weakly modified by the electrostatic force induced by an excess charge $q = e$. This condition holds for a small enough voltage bias V (and a correspondingly

small effective electric field \mathcal{E}) when the shift of the nanotube equilibrium position due to a single excess charge, $d_n = e\mathcal{E}/(M\omega_n^2)$, is small on the scale of the tunneling length, *i.e.* when $d_n/\lambda \ll 1$. In this limit the onset of a shuttle instability occurs independently in the different vibration modes [7] and if $\omega \ll \Gamma$ the instabilities are soft [21], *i.e.* the amplitude A_n of stationary shuttle vibrations goes to zero as \mathcal{E} approaches a critical field $\mathcal{E}_c = 4\Gamma\lambda\gamma M/e$ from above. For small enough positive values of $\mathcal{E} - \mathcal{E}_c$ the vibration amplitudes A_n will therefore be small compared to the tunneling length λ and one may expand in the small parameter A_n/λ . By keeping third order terms one captures the most important non-linear effects.

Now we analyze Eqs. (1) and (2) in the limits discussed above. A formal solution of Eq. (2) is

$$p(t) = \sum_{m=0}^{\infty} (-\Gamma(x)^{-1} \partial_t)^m \Gamma_L(x)/\Gamma(x) \quad (3)$$

which is a series expansion in the small parameter ω/Γ . If $\omega_n \ll \Gamma$ for all modes n it is sufficient to retain only the first order term and substitute the truncated solution into Eq. (1). After expanding to third order in the displacements x_n , the resulting non-linear equations for x_n are solved by choosing the Ansatz: $x_n(t) = \lambda A_n(t) \sin(\omega_n t + \chi_n(t))$ and by then averaging over the fast oscillations [22]. The remaining equations describe the slow time variation of the amplitudes A_n and phases χ_n of the vibrations ($\dot{A}_n, \dot{\chi}_n \ll \omega_n$). Since the oscillator frequencies ω_n are incommensurable (see above) the amplitude and phase equations are decoupled in the limit considered here. Then the amplitude equations are

$$\dot{A}_n = \alpha_n A_n (\delta_n - A_n^2 - 2 \sum_{m \neq n} A_m^2), \quad (4)$$

with

$$\delta_n = 16 \left(1 - \frac{4\gamma\Gamma\lambda}{\omega_n^2 d_n} \right) + \mathcal{O}\left(\frac{\omega_n^2}{\Gamma^2}\right), \quad \alpha_n = \frac{d_n \omega_n^2}{128\lambda\Gamma} \left[1 + \mathcal{O}\left(\frac{\omega_n^2}{\Gamma^2}\right) \right]$$

One notes from the expression of d_n that the product $\omega_n^2 d_n$ does not depend on n and that therefore δ_n and α_n in Eq. (4) do not depend on n to leading order in ω_n/Γ . This will be used in the following analysis and allows us to write $\alpha_n = \alpha$ and $\delta_n = \delta$. The relevance of corrections to these values will be discussed later.

A complete analysis of how the solutions to Eq. (4) evolve is possible when two modes n, m are unstable. In this case one has two non-linear first order differential equations and the stationary points can be classified using standard techniques. The stationary points found and their classification are listed in Table I and the phase space is shown in Fig. 2. We find that the stationary solution corresponding to finite amplitude vibrations of both modes is a saddle point and the solutions describing finite amplitude vibrations of one mode and

$\{A_1, A_3\}$	Type
$\{0, 0\}$	Repulsive fixed point
$\{0, \sqrt{\delta}\}$	Attractive fixed point
$\{\sqrt{\delta}, 0\}$	Attractive fixed point
$\{\sqrt{\delta/3}, \sqrt{\delta/3}\}$	Saddle point

Table I: Classification of stationary points when two modes ($n=1$ and 3) are included and both are unstable ($\delta > 0$). Four stationary points where $A_1, A_3 \geq 0$ are found. Two of them are attractors and correspond to only one unstable mode, the other being stable. Which mode is unstable is determined by the initial conditions.

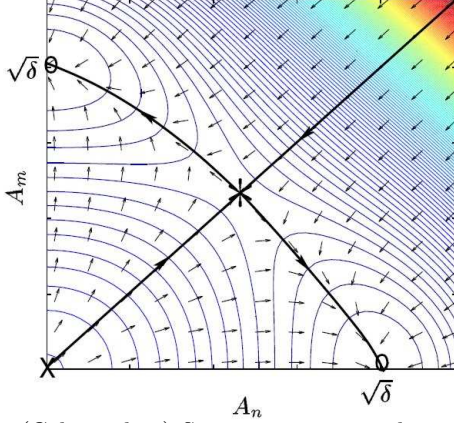


Figure 2: (Color online) Stationary points when two modes (n and m) are unstable. Two attractors, indicated by (•), correspond to a finite amplitude of one mode while the other mode is suppressed. The stationary point marked with (x) is a repeller and the point indicated by (*) is a saddle point. The thick lines are separatrices that trajectories cannot cross. The separatrix $A_n = A_m$ ensures that if $A_n(0) > A_m(0)$, this inequality hold for all times t .

zero amplitude of the other are attractive fixed points. This means that depending on the initial conditions, one mode is selected to vibrate with finite amplitude while vibrations in the other mode are suppressed. Although a complete analysis of the general non-linear problem can not be done, a general statement for a system with $N > 2$ modes can be formulated for small δ . In this limit one finds that the N coupled non-linear equations (4) are characterized by N stable fixed points in the vector space $\vec{A} = \{A_n\}$. The evolution of the system in this space is represented by the motion of the point $\vec{A}(t)$ along a certain trajectory. The stable points are given by $\vec{A}_l(\infty) = (A_l(\infty) = \sqrt{\delta}, A_{n \neq l}(\infty) = 0)$, corresponding to one mode vibrating with amplitude $\sqrt{\delta}$ and all other modes having zero amplitude. More precisely we have proven the following theorem: if the initial conditions are such that $A_l(0) > A_{n \neq l}(0)$, then the amplitude $A_l(t)$ increases monotonically towards the final value $A_l(\infty) = \sqrt{\delta}$ while the other amplitudes $A_{n \neq l}(t)$ decay exponentially towards zero as $t \rightarrow \infty$. The asymptotic estimate $A_{n \neq l}(t) \leq \sqrt{\delta} \exp\{-\alpha t(A_l^2(0) - A_n^2(0))\}$

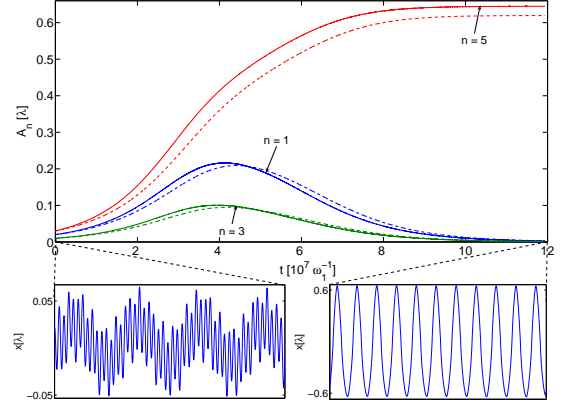


Figure 3: (Color online) Nanotube vibration amplitude as a function of time when three modes ($n = 1, 3, 5$) are unstable ($\delta > 0$) and included in a full numerical solution of Eqs. (1)-(2) with $\gamma/\omega_1 = Q_1^{-1} = 6.1 \times 10^{-6}$, $d_1/\lambda = 0.01$, $\omega_1/\Gamma = 0.0025$ and initial conditions $A_1(0) = 0.02$, $A_3(0) = 0.01$, $A_5(0) = 0.03$. These parameters were chosen to allow a comparison with the approximate result of Eq. (4) which is plotted as dashed curves. The lower left panel shows the quasi-periodic oscillation of the nanotube center position just after the onset of the instability, while the lower right panel shows the regular vibrations that appear after all but the $n=5$ mode amplitudes have been suppressed (see text).

gives an upper limit to the decaying amplitudes. The theorem guarantees a remarkable feature of the shuttle instability in that it allows a selective amplification of one of the normal modes of the shuttle vibrations. Initially quasi-periodic vibrations (for incommensurable frequencies ω_n) are forced to self-organize into regular large-amplitude vibrations with a frequency corresponding to that of a single normal mode.

We now resort to a numerical analysis in order to verify and generalize the analytical results obtained above. We begin by using the same parameter range as before, *i.e.* we choose parameters in order to allow a comparison between the numerical and analytical results rather than to model realistic experiments. We will then show that the same type of behaviour obtains for more realistic sets of parameters, for which no analytic solutions is available. Figure 3 shows numerical and analytical results for the time evolution of the vibration amplitude when there are three different unstable mechanical modes ($n=1, 3, 5$). It is clear that even though all three modes initially increase their amplitudes, a single mode is selected and the other modes are suppressed at large times. Here the $n=5$ mode initially had the largest deviation and hence the vibration frequency in the stationary state is given by ω_5 . Similar figures when modes $n=1$ or 3 ends up with a finite amplitude can be obtained by changing the initial conditions.

So far we have only discussed cases when the final vibration amplitude is smaller than the tunneling length λ . Numerically, we have also investigated the opposite situ-

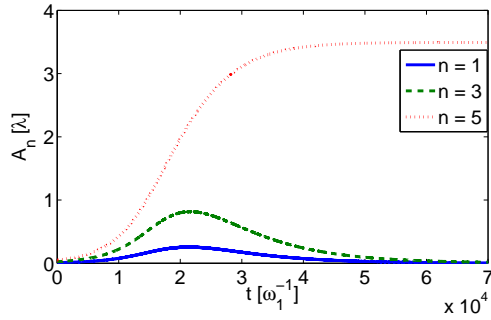


Figure 4: (Color online) Time evolution of the vibration amplitude obtained from a numerical solution of Eqs. (1)-(2) when three modes ($n = 1, 3, 5$) are unstable and $\gamma/\omega_1 = Q_1^{-1} = 5.5 \times 10^{-4}$, $d_1/\lambda = 0.7$ and $\omega_1/\Gamma = 0.005$. The initial conditions were $A_1(0) = 0.005$, $A_3(0) = 0.0025$ and $A_5(0) = 0.01$. The large amplitudes make an approximate analysis based on Eq. (4) invalid, but the phenomenon of a selective excitation persists even in this case — the mode with the largest initial deviation is selected to end up with a large vibration amplitude.

ation and found results that are qualitatively similar. As an example, a full numerical solution of Eqs. (1) and (2) for a case when the final amplitude exceeds λ is shown in Fig. 4.

Finally we discuss the coefficients α_n and δ_n . In the previous analysis we used the approximation that these coefficients are the same for all modes, which is only valid when $\Gamma \gg \max \omega_n$ and the dissipation mechanism affects all the modes in the same way. In general if one takes corrections of order ω_n^2/Γ_n^2 into account or considers a mode-dependent dissipative mechanism, one has $\delta_n \neq \delta_m$. This breaks the symmetry between the modes and leads to a situation where the final vibration state is not simply determined by the largest initial vibration mode amplitude. In this case the number of stable attractors can be smaller than the number of unstable modes. This implies that in some cases, even though a mode is initially unstable, it cannot reach finite amplitude vibrations since it is suppressed by another mode.

In conclusion we have investigated electromechanical instabilities of different mechanical vibration modes of a suspended carbon nanotube. We have shown that the excitation mechanism considered leads to a selective excitation of a specific mode depending on the initial condi-

tions. This demonstrates a way of using local tunneling injection of charge to probe the mechanics of extended nano-objects. The analysis presented here can be generalized to apply to other multi-mode shuttle structures. The phenomenon of a selective excitation of a specific mode is general in the sense that even though several modes are unstable, only a single mode reaches a steady state with a finite amplitude.

Stimulating discussions with A. Isacsson and financial support from the Swedish VR and SSF and from the EC (FP6-003673, CANEL) is gratefully acknowledged.

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